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Is Dodecahedral P_{20} Special?

Hu, Ching-Han; Shen, M. ; Schaefer, H. F.

The laboratory study of phosphorus clusters by laser-based mass spectrometric methods indicates, tentatively, that P_{21}^{+} may be special. A plausible interpretation might place a P^{+} ion interior to a dodecahedral P_{20} molecule.*Ab initio* quantum mechanical methods have been applied to the P_{20} molecule using contracted gaussian basis sets as large as (9*s* 6*p* 4*d* 3*f*) on each phosphorus atom. At the highest level of theory, dodecahedral P_{20} is predicted to lie 23 kcal/mol above five separated P_4 molecules.

Key words： Phosphorus clusters - P_{20} - Dodecahedra